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Three-dimensional Structure of Nanoparticles from High-energy X-ray Diffraction and Atomic Pair Distribution Function Analysis VALERI PETKOV, Dept. Physics, Central Michigan University — Knowledge of the atomic-scale structure is an important prerequisite to understand and predict the properties of materials. In the case of crystals it is obtained from the positions and intensities of the Bragg peaks in the diffraction patterns. However, materials constructed at the nanoscale lack the translational symmetry and long-range order of perfect crystals. The diffraction patterns of such materials show only a few Bragg peaks, if any, and a pronounced diffuse component. This poses a real challenge to the usual techniques for structure characterization. The challenge can be met by employing the so-called atomic Pair Distribution Function (PDF) technique and high energy x-ray diffraction. This non-traditional experimental approach takes into account both Bragg and diffuse scattering and yields the atomic structure in terms of a small set of parameters such as a unit cell and atomic coordinates. The basics of the technique will be introduced and its potential demonstrated with results from recent structural studies gold, ZrO_2 and GaN nanoparticles.

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